

Phosphonic acid, bis(1-methylethyl) ester  
1809-20-7 | DTXSID7061988

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.08e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.76e-01

Confidence level: 5.21e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Emylcamate</div> <div>Measured: 7.24e-02</div> <div>Predicted: 3.35e-01</div>	<div>Image not found</div> <div>Hexamethylphosphoramide</div> <div>Measured: 1.33e-02</div> <div>Predicted: 7.54e-02</div>	<div>Image not found</div> <div>Furan, 2,3-dihydro-</div> <div>Measured: 2.77e-01</div> <div>Predicted: 200</div>
<div>Image not found</div> <div>Aspirin</div> <div>Measured: 5.79e-01</div> <div>Predicted: 1.03e-05</div>	<div>Image not found</div> <div>Methoprotryne</div> <div>Measured: 4.52</div> <div>Predicted: 6.52e-07</div>	